

Chemistry 658 Crystallography

Fall, 2006

TR noon - 1:15 p.m., Bilger 341C

Instructor: Karl Seff, ext. 67665, seff@hawaii.edu

This is the last time that this course will be taught by this instructor.

Texts: International Tables for Crystallography, Brief Teaching Edition of Volume A, Space Group Symmetry.
Handout: Azároff, Elements of X-ray Crystallography, Chapter 1 and Chapters 3 to 11.
Additional handouts.

The following topics will be covered:

Elementary crystallographic point symmetries, Hermann-Mauguin notation

Generation of elementary plane groups

Crystal systems, Miller indices

Generation of most plane groups

Bravais lattices and their transformation

Glide planes, screw axes, space groups

Properties of X-rays, Bragg's Law

X-ray source spectra, effect of structure on diffraction intensities

The determination of the structure of NaCl, as it was first done

Precision in wavelength measurement, X-ray absorption

The reciprocal lattice

Bragg's Law in reciprocal space

Reciprocal space representations of diffraction, the Ewald sphere

Diffraction by a 1D, 2D, and 3D grating, Laue's equations

Atomic scattering factors

Anomalous dispersion, corrections for and absolute configuration determination

Scattering from amorphous or partly amorphous samples

Derivation of the diffraction equation for a perfect crystal

The structure factor and systematic absences

Determination of lattice symmetry and space groups

Extinction, double reflection, mosaic crystals and integrated intensities

The effect of temperature on structure factors

Collection of diffraction data

Diffraction from a polycrystalline sample

Structure factor calculation

Preliminary investigation of a crystal--laboratory procedures

Common space groups, determination of easy crystal structures

The 3D electron-density function and its relation to the structure factor

The phase problem, Fourier syntheses

The heavy atom method--simple cases

Calculation of the number of unique reflections

The Direct Method for phase determination

Sayre's equation and examples of its application

Hour examinations: There will be three.

Final Examination: Thursday, December 14 at noon

Grading: Each hour exam: 20%; Final: 40%; Homework will be used to decide "borderline" course grades.